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Density and viscosity of biodiesel as a function of temperature: Empirical models

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Biodiesel is a promising alternative of renewable energy obtained from natural raw material. This work presents empirical models to predict the density (ρ) and dynamic viscosity (μ) of fatty acid methyl esters (FAMEs), biodiesel, and biodiesel blends in a wide range of temperature. The average absolute deviation (AAD) was 0.43% in density, and 6.39% in viscosity.

Contents

1. Introduction

As a result of the population growing, it could be expected in the near future a greater consumption of energy, faster depletion of petroleum oil reserves, increase in fossil fuel prices, and enactment of more stringent environmental standards. The above events can be considered as driving forces that encourage the use of renewable energies.

Biodiesel is presented as an attractive renewable energy that can be used as additive of fossil diesel. Current biodiesel production is carried out by trans-esterification, a process in which triglycerides of vegetable oils or animal fats reacts with alcohol to be converted into alkyl-esters and glycerin [1–7].

Recently, the production and use of biodiesel has been increasing around the world [1]. For instance, the global biodiesel production was 204 (2001), 250 (2002), 338 (2003), 666 (2004), 2162 (2005), 5963 (2006), 11663 (2007), and 16251 (2008) thousand barrels, according to the U.S. Energy Information Administration. Therefore, the increase in the biodiesel production is expected to be continuing in the coming decades.

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Nomenclature

FAME	fatty acid methyl ester
T	temperature, K
M	molecular weight, g/mol
N	number of double bonds in the fatty acid chain
n_{exp}	Number of experimental points
ANOVA	analysis of variance
DF	degrees of freedom
ρ	density, g/cm^3
μ	dynamic viscosity, mPa s
AAD	average absolute deviation, %
D	deviation or relative error, %

Each country is looking for vegetable oils that are best suited to the climatic and soil conditions belonging to each geographic region. For instance, soybean oil in the U.S., rapeseed and sunflower oils in Europe, and palm oil in Southeast Asia (mainly Malaysia and Indonesia) [8]. In addition, among the reasons to use biodiesel fuels, their environmental sustainability (including life-cycle greenhouse emissions) should be considered nowadays. Sustainable directives published by governments worldwide have promoted the use of biodiesel fuels derived from waste oils or fats.

Biodiesel has many benefits, including renewability, non-toxicity, low flammability (that makes biodiesel safer regarding to the storage and transportion because its flash point varies from 415 to 463 K [2]), inherent lubricity, and biodegradability (biodiesel is as biodegradable as sugar, biodiesel degrades about four times faster than diesel [3]); also it is safe for use in all conventional diesel engines and virtually without sulfur and aromatics [4,9]. However, disadvantages of biodiesel with regard to fossil diesel are higher viscosity (*v.g.* the kinematic viscosity of biodiesel at 313 K is in the range of 3.6 to 5.0 cSt, whereas it is 1.9 to 3.8 cSt for diesel [3]), lower energy content (biodiesel has a higher heating value (*HHV*) from 39.3 to 39.8 MJ/kg, whereas diesel has a *HHV* from 45.3 to 46.7 MJ/kg [3]), higher cloud point (262–289 K for biodiesel and 256–265 K for diesel [3]), higher pour point (258–286 K for biodiesel and 237–243 K for diesel [3]); its main disadvantage is the current high cost of some raw material required to produce it [3,5].

The biodiesel quality is governed by international standards, for instance, in Europe the biodiesel fuel standards are compiled in the Norm CEN EN 14214 and in United States of America in the Norm ASTM D6751 [6,7]. Density and viscosity of biodiesel are two important physical properties because they are widely used in combustion models, design–operation–control of processes, and fuel quality.

Substance density is defined as its mass per unit volume. Density is a physical property that can be used to calculate the precise volume of fuel necessary to supply an adequate combustion. The injection system, formed by high-pressure pump and injectors, enters to the cylinder a discrete volume of fuel, which is calculated by the Electronic Control Unit of the vehicle depending on the driving conditions [10]. The density of fuels mainly affects the spray momentum and the distribution of equivalence ratio. Apart of that, density is commonly used in numerous unit operations of biodiesel production. Also, density values are required to properly design: reactors, distillation units, storage tanks, and pipes [7].

The physical property of substances that characterized their resistance to flow is the viscosity. The viscosity of biodiesel is slightly greater than that of petro-diesel (for instance, 1.55 times more higher, for the case of the sunflower biodiesel versus petro-diesel, according to the results reported by Parente et al. [11]. On the other hand, the viscosity of biodiesel is an order of magnitude less than that of the parent vegetable oil or fat [12]. Although fuel spray penetration into the combustion chamber can be eventually promoted by higher viscosities of fuels, there are more adverse effects that can occur in the engine performance, because a higher viscosity can cause excessive fuel injection pressures for the engine warm-up, increasing the energy demand of pumps and tending to form larger droplets up, leading to a poorer spray. Those phenomena can cause an incomplete combustion, wear of the fuel pump elements, choking of the fuel injectors, and ring carbonization. [8,13–17]. Apart of that, the viscosity is important in the design of the equipment to be used in industry as pipes, fittings, and distillation columns. Also it is required for monitoring the quality of fuels [6,18].

Density and viscosity of biodiesel depend on the alkyl esters profile and in consequence on the raw materials used for its production [6]. Although several methods are available for predicting the density and viscosity of petroleum-based fuels with a dependence on temperature. In contrast, there are few methods for biodiesel [19]. Even more, in the particular case of biodiesel, several works are only limited to predict these properties at fixed temperatures, for instance, 288.15 K for density and 313.15 K for kinematic viscosity. The above behavior could be due to the influence of the ASTM D6751 standard that specifies the conditions that must be fulfilled to define the quality of biodiesel. However, the need for reliable models that can incorporate the dependence on temperature is of great importance, because they could eventually be used by biodiesel processes, as well as for the development of better combustion models.

Both Baroutian et al. and Veny et al. [20,21] were using the Janarthanan empirical method and the Spencer and Danner model to predict the jatropha and palm biodiesel density at different temperatures with reasonably good accuracy. In 2010, Anand et al. were proposed a methodology based on the modified Rackett equation to predict the density of thirteen biodiesel samples from vegetable oils at 288.15 K [22]. More recently, in 2011 Pratas et al. proposed a methodology based on Kay's mixing rule and the group contribution method for predicting the density of ten biodiesel samples at different temperatures [7].

On the other hand, the Vogel equation was used by Yuan et al. in 2005 and 2009 to correlate the viscosity of some biodiesel samples with temperature [13,14]. Shu et al. were developing in 2007 a method to predict the viscosity of biodiesel based on the topological index [23]. Freitas et al. were using a viscosity database to evaluate four models, which were able to predict biodiesel viscosity at different temperatures (the models were named by those authors as Ceriani, Krisnangkura, Yuan and revised Yuan) [15]. Parente et al. estimated the viscosity for the sunflower biodiesel and fish biodiesel by using three models (Thomas, Orrick–Erbar, and modified Sastri–Rao) [11]. do Carmo et al. [19] made the comparison of five models (identified as Ceriani, Yuan, revised Yuan, one-fluid and two-fluid) predicting the viscosity as a function of temperature of thirty one pure biodiesel samples and four biodiesel blends.

Given the importance of reliable prediction models, the main objective of this work will be to develop empirical models that are able to predict both the biodiesel's density and biodiesel's viscosity as a function of methyl ester concentration and temperature. In order to achieve the above purpose, we will do the

following steps: (a) robust experimental databases will be compiled for both the density and viscosity of methyl esters in a wide range of temperature, (b) relationships between variables will be sought (density and viscosity of methyl esters as dependent variables; length of the fatty acid chain, number of double bonds, and temperature as independent variables, (c) empirical models will be developed for the physical properties of methyl esters, which will be tested and validated, (d) mixing rules combined with the FAME empirical models will be used to develop a methodology to predict both the density and viscosity of biodiesel, and (e) capability of prediction of our models will be confronted with some ones previously reported in the literature.

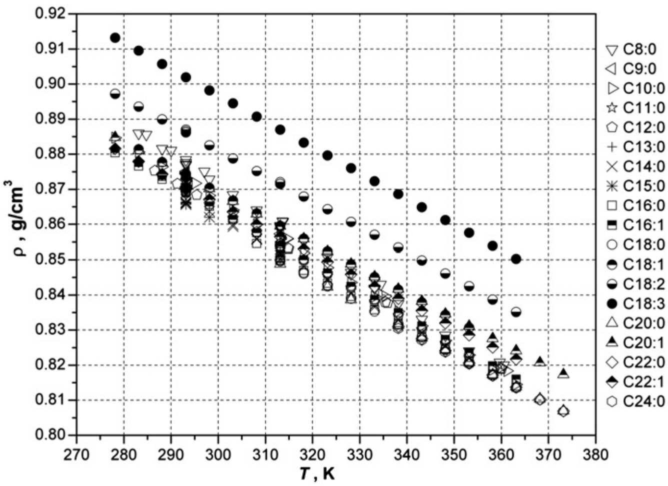


Fig. 1. Effect of temperature on the methyl ester density.

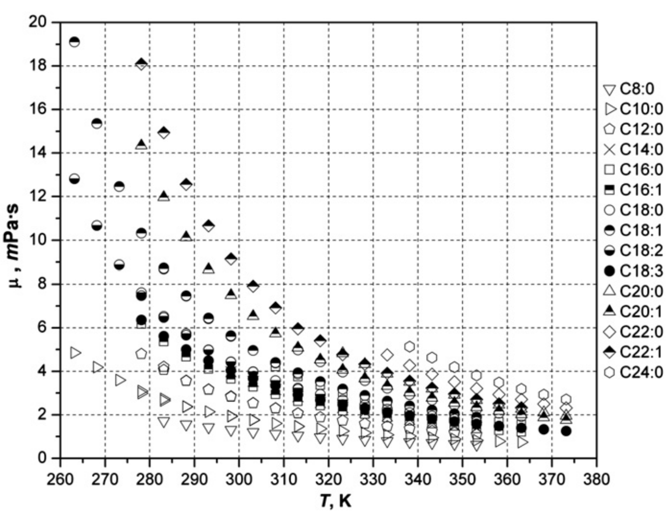


Fig. 2. Effect of temperature on the methyl ester dynamic viscosity.

2. Models

This section presents the main steps that were approached to develop the models of density and viscosity of methyl esters and biodiesel, which can be summarized as: accumulation and selection of the experimental data from literature, search for functionality between variables, and optimization of parameters.

2.1. Databank

The experimental data of density (351 points) and dynamic viscosity (259 points) compiled in this work are presented as a function of temperature by Figs. 1 and 2. It can be seen from Fig. 1 that the density of FAMEs decreases linearly as temperature increases. An increase in temperature causes more molecular motion due to the increase on the kinetic energy, therefore, the molecular weight per unit volume decreases, and by consequence density decreases. Densities of FAMEs with similar number of carbon atoms increase with increasing the number of double bonds (for instance, $\rho_{C18:3} > \rho_{C18:2} > \rho_{C18:1} > \rho_{C18:0}$). We can observe a strip of negative slope in Fig. 1 at which experimental densities are agglomerated and some ones overlapping for a given temperature. In contrast, the densities for the C18:2 and C18:3 methyl esters are further away from that strip.

An increase in the temperature leads to a reduction in the dynamic viscosity of FAMEs (Fig. 2) by means of a non-linear behavior. Generally, in the liquid occurs that cohesive forces between the molecules dominate the molecular momentum transfer. As the temperature increased, also increases the average kinetic energy of molecules, due to a decrease in the attractive forces that hold the molecules together. In addition, as the temperature increased, the instant slope of each FAME decrease, being the FAMEs of lower molecular which have more significant

Table 1
Database for experimental FAME density.

Reference	Fatty acid	Methyl ester name	Methyl ester formula	*M* (g/mol)	*N*	n_{exp}	Temperature range (K)
[6,10,24,25]	C8:0	Methyl caprylate	$C_9H_{18}O_2$	158.2380	0	33	[283.15, 360.55]
[10,24]	C9:0	Methyl pelargonate	$C_{10}H_{20}O_2$	172.2646	0	6	[293.15, 313.15]
[6,10,24,25]	C10:0	Methyl caprate	$C_{11}H_{22}O_2$	186.2912	0	36	[278.15, 363.15]
[10,24]	C11:0	Methyl undecanoate	$C_{12}H_{24}O_2$	200.3178	0	5	[293.15, 313.15]
[6,10,24,25]	C12:0	Methyl laurate	$C_{13}H_{26}O_2$	214.3443	0	36	[283.15, 360.05]
[10,24]	C13:0	Methyl tridecanoate	$C_{14}H_{28}O_2$	228.3709	0	5	[293.15, 313.15]
[6,10,24,26]	C14:0	Methyl myristate	$C_{15}H_{30}O_2$	242.3975	0	28	[293.15, 353.15]
[10,24]	C15:0	Methyl pentadecanoate	$C_{16}H_{32}O_2$	256.4241	0	8	[293.15, 313.15]
[6,10,24]	C16:0	Methyl palmitate	$C_{17}H_{34}O_2$	270.4507	0	15	[308.15, 363.15]
[27]	C16:1	Methyl palmitoleate	$C_{17}H_{32}O_2$	268.4348	1	18	[278.15, 363.15]
[6,10,24,26]	C18:0	Methyl stearate	$C_{19}H_{38}O_2$	298.5038	0	22	[313.15, 363.15]
[6,10,24]	C18:1	Methyl oleate	$C_{19}H_{36}O_2$	296.4879	1	26	[283.15, 353.15]
[6,10,24]	C18:2	Methyl linoleate	$C_{19}H_{34}O_2$	294.4721	2	22	[278.15, 363.15]
[27]	C18:3	Methyl linolenate	$C_{19}H_{32}O_2$	292.4562	3	18	[278.15, 363.15]
[6,10,24]	C20:0	Methyl arachidate	$C_{21}H_{42}O_2$	326.5570	0	12	[313.15, 373.15]
[27]	C20:1	Methyl gadoleate	$C_{21}H_{40}O_2$	324.5411	1	20	[278.15, 373.15]
[27]	C22:0	Methyl behenate	$C_{23}H_{46}O_2$	354.6101	0	8	[338.15, 373.15]
[10,24,27]	C22:1	Methyl erucate	$C_{23}H_{44}O_2$	352.5943	1	25	[278.15, 363.15]
[27]	C24:0	Methyl lignocerate	$C_{25}H_{50}O_2$	382.6633	0	8	[338.15, 373.15]

Table 2
Database for experimental FAME dynamic viscosity.

Reference	Fatty acid	Methyl ester name	Methyl ester formula	M (g/mol)	N	n_{exp}	Temperature range (K)
[6]	C8:0	Methyl caprylate	$C_9H_{10}O_2$	158.2380	0	15	[283.15, 353.15]
[1,6]	C10:0	Methyl caprate	$C_{11}H_{22}O_2$	186.2912	0	29	[263.15, 363.15]
[1,6]	C12:0	Methyl laurate	$C_{13}H_{26}O_2$	214.3443	0	23	[278.15, 353.15]
[6]	C14:0	Methyl myristate	$C_{15}H_{30}O_2$	242.3975	0	12	[298.15, 353.15]
[6]	C16:0	Methyl palmitate	$C_{17}H_{34}O_2$	270.4507	0	12	[308.15, 363.15]
[27]	C16:1	Methyl palmitoleate	$C_{17}H_{32}O_2$	268.4348	1	18	[278.15, 363.15]
[6]	C18:0	Methyl stearate	$C_{19}H_{38}O_2$	298.5038	0	11	[313.15, 363.15]
[1,6]	C18:1	Methyl oleate	$C_{19}H_{36}O_2$	296.4879	1	26	[263.15, 353.15]
[1,6]	C18:2	Methyl linoleate	$C_{19}H_{34}O_2$	294.4721	2	27	[263.15, 353.15]
[27]	C18:3	Methyl linolenate	$C_{19}H_{32}O_2$	292.4562	3	20	[278.15, 373.15]
[27]	C20:0	Methyl arachidate	$C_{21}H_{42}O_2$	326.5570	0	11	[323.15, 373.15]
[27]	C20:1	Methyl gadoleate	$C_{21}H_{40}O_2$	324.5411	1	20	[278.15, 373.15]
[27]	C22:0	Methyl behenate	$C_{23}H_{46}O_2$	354.6101	0	9	[333.15, 373.15]
[27]	C22:1	Methyl erucate	$C_{23}H_{44}O_2$	352.5943	1	18	[278.15, 363.15]
[27]	C24:0	Methyl lignocerate	$C_{25}H_{50}O_2$	382.6633	0	8	[338.15, 373.15]

instant slope decreasing. On the other hand, for a given temperature, the viscosity of FAMEs increased with molecular weight but decreased with increasing the number of double bonds (for instance, $\mu_{C18:3} < \mu_{C18:2} < \mu_{C18:1} < \mu_{C18:0}$).

Tables 1 and 2 indicate the source from which the experimental data of density (Fig. 1) and viscosity (Fig. 2) were tacked out (numerical values are not included because they are available on the cited references). The number of the experimental points and the range of temperature are also included. Small dispersion and a wide range of temperature were the main factors taken into account to select the experimental data.

2.2. Empirical models for methyl esters

Empirical correlations were derived using a methodology similar to that of a previous work [28]. But now it was included the temperature dependence, see Eqs. (1) and (2). It must be noted that nineteen FAMEs (351 experimental points) for the density (Table 1) and fifteen FAMEs (259 experimental points) for the dynamic viscosity (Table 2) were taken into account to optimize the corresponding parameters of Eqs. (1) and (2).

$$\rho = 1.069 + \frac{3.575}{M} + 0.0113N - 7.41 \times 10^{-4}T \quad (1)$$

$$\ln\mu = -18.354 + 2.362 \ln M - 0.127N + \frac{2009}{T} \quad (2)$$

in which M is the FAME's molecular weight in g/mol, N is the number of double bonds present in the fatty acid chain, and T is the temperature in K.

2.3. ANOVA for empirical models

Desing-Expert v.6 was used for the regression by means of the two-level-factorial method. Levels of factors are reported in Tables 3 and 4. The low and high levels for the $1/M$ factor correspond to the reciprocal molecular weight of the methyl lignocerate and methyl caprylate, respectively. In this work, it was proposed that the viscosity of FAME varies in a logarithmic way with its molecular weight. Therefore, the $\ln M$ factor was restricted between 5.06 and 5.95, which correspond to the natural logarithm of the molecular weight of the methyl caprylate and methyl lignocerate, respectively. The N factor was limited in the range of 0 to 3, both for correlations of density and viscosity, because in most of the biodiesel samples produced from vegetable oils, the concentration of methyl esters with four or more double bounds in the fatty acid chain is negligible (Eqs. (1) and (2) should be used with caution in the case of some biodiesel samples from fish oil, because they could contain methyl esters with four double bonds).

Table 3
Factors and levels for full factorial design of density.

Factor	Low level	High level
$1/M$	2.613×10^{-3}	6.32×10^{-3}
N	0	3
T	278.15	373.15

Table 4
Factors and levels for full factorial design of viscosity.

Factor	Low level	High level
$\ln M$	5.06	5.95
N	0	3
$1/T$	2.68×10^{-3}	3.8×10^{-3}

Table 5
Analysis of variance (ANOVA) for the regression model equation and coefficients.

	Sum of squares	Degrees of freedom (DF)	Mean square	F-value	Prob > F
Model: Density					
Regression	0.16	3	0.054	7632.48	< 0.0001
Residual	2.431×10^{-3}	346	7.026×10^{-6}		
Total, corrected	0.16	349			
Model: Dynamic viscosity					
Regression	108.29	3	36.1	4882.44	< 0.0001
Residual	1.89	255	7.393×10^{-3}		
Total, corrected	110.18	258			

Based on a 95% confidence level, the model was tested to be significant, as the computed F value (7632.48 for the density model and 4882.44 for the viscosity model) are much higher than the theoretical $F0.05$ value (2.6 for both density and viscosity models, this value is reported for three degrees of freedom and residual higher than 120). On the other hand, values of "Prob > F" less than 0.05 indicate model terms are significant. In this case ($1/M$, N and T for the density model; $\ln M$, N and $1/T$ for the viscosity model) are significant model terms (Table 5). Thus, from

these statistical tests, it was found that the empirical models are adequate for predicting the density and viscosity of FAME within the range of variables studied.

2.4. Biodiesel models

Many of the scientific publications relating to biodiesel have been reported the FAME profile on a mass base (*v.g.* mass fraction or weight percent) [11,14,29–32]. However, there are some works that have been used a mol base (*v.g.* mol fraction or mol percent) [20,21,33]. Therefore, it seems a good idea to have a procedure to convert a given representation of concentration in other; the mol fraction can be converted into mass fraction by means of the Eq. (3), whereas the mass fraction can be converted into mol fraction by means of the Eq. (4).

$$w_i = \frac{x_i M_i}{\sum_{i=1}^{n} x_i M_i} \tag{3}$$

$$x_i = \frac{\frac{w_i}{M_i}}{\sum_{i=1}^{n} \frac{w_i}{M_i}} \tag{4}$$

where x_i, w_i and M_i are the mol fraction, mass fraction, and molecular weight of the *i*th FAME, respectively.

The density of biodiesel could be calculated by means of Eq. (5) (Kay's mixing rule), we are assuming the absence of excess volume at blending because biodiesel is a simple mixture composed, in general, by less than ten fatty acid alkyl esters, and consequently, it is close to that an ideal mixture [7]. In a previous work Ramírez–Verduzco et al. [28] found that the representation in mol fraction or mass fraction has a marginal impact on the prediction of the biodiesel density due to the similarity in the nature and size of the compounds present in the biodiesel. A similar observation was reported by Pratas et al. [7]. By the foregoing and by our convenience, in this work only will be used the mass fraction for the Kay's rule.

$$\rho_b = \sum_{i=1}^{n} w_i \rho_i \tag{5}$$

where w_i and ρ_i are the mass fraction and density in g/cm^3 of the *i*th FAME and ρ_b represents the density of biodiesel in g/cm^3.

The viscosity of biodiesel could be estimated by means of Eq. (6). This is a simplification of the Grunberg–Nissan equation at which the interaction term of binary pairs of methyl esters has been neglected. Although the Grunberg–Nissan equation was originally developed considering the mol fraction mol as weighting factor, in this work was chosen the mass fraction due that it is the most widely way to report the concentration of biodiesel in the literature, and similarly to the density, the prediction of the biodiesel viscosity is indistinguishable to the use of the mol fraction or mass fraction, as it has been previously observed by Ramírez–Verduzco et al. [28].

$$\ln\mu_b = \sum_{i=1}^{n} w_i \ln\mu_i \tag{6}$$

where w_i and μ_i are the mass fraction and dynamic viscosity in mPa s of the *i*th FAME and μ_b represents the dynamic viscosity of biodiesel in mPa s.

Eqs. (5) and (6) require prior knowledge of the experimental physical properties for each compound (FAME) to estimate the properties of the mixture. Furthermore, they must be evaluated at the same temperature of the biodiesel, which as we know, they are obtained after much effort. In this work, we provide a useful solution of the problem by replacing Eq. (1) in Eqs. (5) and (2) in Eq. (6), respectively.

$$\rho_b = \sum_{i=1}^{n} w_i \left(1.069 + \frac{3.575}{M_i} + 0.0113 N_i - 7.41 \times 10^{-4} T\right) \tag{7}$$

where w_i, M_i, N_i are the mass fraction, molecular weight in g/mol, and the number of double bonds in the fatty acid chain, T is the temperature in K, and ρ_b is the density of biodiesel in g/cm^3.

$$ln\mu_b = \sum_{i=1}^{n} w_i \left(-18.354 + 2.362 \ln M_i - 0.127 N_i + \frac{2009}{T}\right) \tag{8}$$

where w_i, M_i, N_i are the mass fraction, molecular weight in g/mol, and the number of double bonds in the fatty acid chain, T is the temperature in *K*, and μ_b is the dynamic viscosity of biodiesel in mPa s.

3. Results and discussion

3.1. FAME's density

Uniform variation on density for the methyl ester homologous series (*v.g.* C8:0, C10:0, C12:0, etc) was observed. The effect of the molecular weight, number of double bonds and temperature on density can be explored by Eq. (1). If we take the FAME C18:0 at 293.15 K as a reference, a density of 0.8638 g/cm^3 can be obtained, if we now change the FAME (and hence, the molecular weight) to C20:0, C22:0 and C24:0, then the density decreases 0.12, 0.22 and 0.31% with respect to the reference; whereas the increase in the number of double bonds by 1, 2 and 3, leads to an increase in the density of 1.33, 2.66 and 3.99%; finally, an increase of the temperature at intervals of 10 K to 303.15, 313.15 and 323.15 K, causes a decrease in the density of 0.85, 1.1 and 2.55%.

Fig. 3 shows the capability of the empirical model to reproduce the experimental density of FAMEs. Very good predictions were obtained because most of the values had a relative error in the range of −0.4 to 0.4%. An average absolute deviation of 0.21% for 351 points was estimated. A maximum deviation of 1.04% at 363.15 K was reached for the methyl palmitoleate compound.

The empirical model of density expressed by Eq. (1) also was validated with experimental information reported by Nevin et al. [34] and Keffler et al. [35]. It is important to mention that those data were not included into the density databank (Table 1) because they were exclusively kept back for validation. Table 6

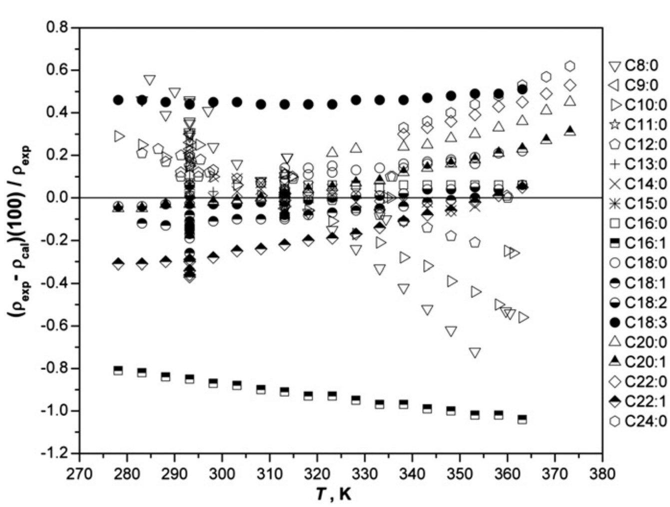


Fig. 3. Comparison between experimental and predicted densities as a function of temperature for saturated and unsaturated FAMEs.

Table 6
Validation of the empirical model of density.

Reference	Fatty acid	Methyl ester name	*M* (g/mol)	*N*	*T* (K)	ρ_{exp} (g/cm^3)	ρ_{cal} (g/cm^3)	*D* (%)
[34]	C8:0	Methyl caprylate	158.238	0	313.15	0.86	0.8595	0.06
					333.15	0.842	0.8447	−0.32
					353.15	0.824	0.8299	−0.72
[34]	C10:0	Methyl caprate	186.2912	0	313.15	0.856	0.8561	−0.01
					333.15	0.84	0.8413	−0.15
					353.15	0.823	0.8265	−0.43
[34]	C12:0	Methyl laurate	214.3443	0	313.15	0.854	0.8536	0.05
					333.15	0.838	0.8388	−0.10
					353.15	0.822	0.824	−0.24
[34]	C14:0	Methyl myristate	242.3975	0	313.15	0.852	0.8517	0.04
					333.15	0.836	0.8369	−0.11
					353.15	0.821	0.8221	−0.13
[34]	C16:0	Methyl palmitate	270.4507	0	313.15	0.85	0.8502	−0.02
					333.15	0.835	0.8354	−0.05
					353.15	0.82	0.8205	−0.06
[34]	C18:0	Methyl stearate	298.5038	0	313.15	0.851	0.8489	0.25
					333.15	0.836	0.8341	0.23
					353.15	0.821	0.8193	0.21
[35]	C18:1	Methyl oleate	296.4879	1	288.15	0.8774	0.8788	−0.16
					293.15	0.8738	0.8751	−0.15
					298.15	0.8702	0.8714	−0.14
					303.15	0.8666	0.8677	−0.13
					333.15	0.845	0.8455	−0.06
					363.15	0.8234	0.8233	0.01

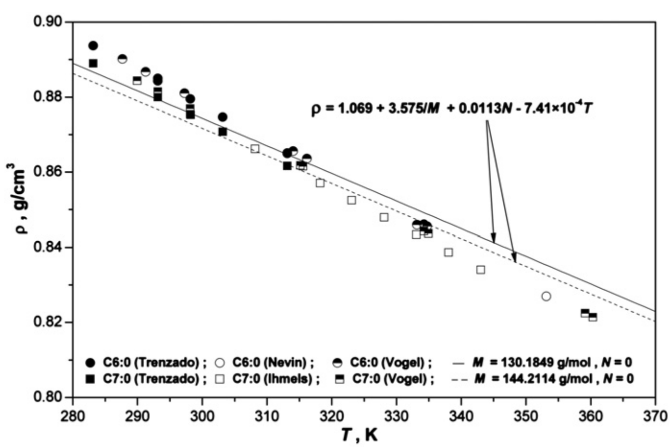


Fig. 4. Extrapolation for the density of FAMEs.

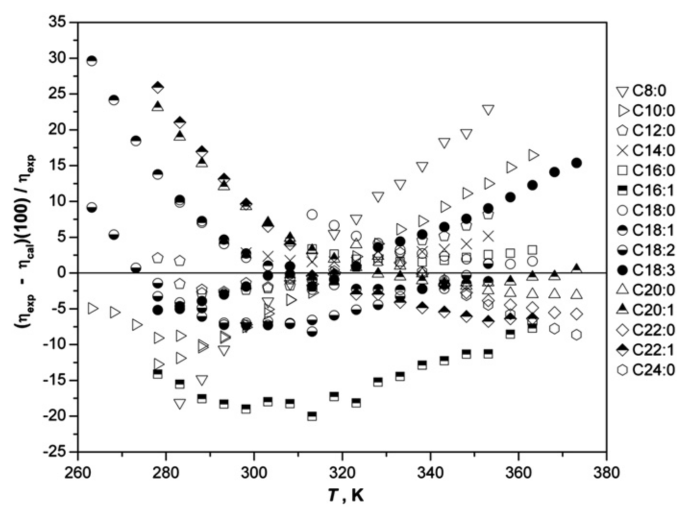


Fig. 5. Comparison between experimental and predicted viscosities as a function of temperature for saturated and unsaturated FAMEs.

shows a comparison between the experimental measurements of density and model predictions of the C8:0, C10:0, C12:0, C14:0, C16:0, C18:0, and C18:1 methyl esters. There were slight differences between the model and experimental results. The higher deviation was 0.72% that corresponds to the C8:0 methyl ester at 353.15 K. The *AAD* was 0.16% for the twenty four points.

On the other hand, it was also tested the model ability for extrapolation by estimating the density of C6:0 and C7:0 methyl esters at different temperatures. Fig. 4 shows a comparison between the model predictions and the experimental data reported by Vogel et al. [25], Nevin et al. [34], Trenzado et al. [36], and Ihmels et al. [37]. The highest deviation was submitted at 353.15 K with the C6:0 methyl ester. The *AAD* was 0.39% for forty extrapolated points.

3.2. FAME's viscosity

The effect of the molecular weight, number of double bonds and temperature on the dynamic viscosity can be explored by means of Eq. (2). Through Eq. (2), a viscosity of 7.1 mPa s it can be estimated for the C18:0 methyl ester at 293.15 K. If we take the value of 7.1 mPa s as reference, an increment of 23.63, 50.2 and 79.8% can be obtained by changing to the C20:0, C22:0 and C24:0 methyl ester. A decrement of 13.33, 24.88 and 34.91% are founded by changing the number of double bonds to 1, 2 and 3. Finally, an increment of 20.23, 35.45 and 47.07% are obtained by changing the temperatures to 303.15, 313.15 and 323.15 K.

Fig. 5 shows the dynamic viscosity deviations between experimental and calculated values of fifteen methyl ester samples at different temperatures. A minimum, maximum and average absolute deviation of 0.09, 29.63 and 6.04%, was reached for 259 analyzed points.

Table 7
Validation of the empirical model of dynamic viscosity.

Reference	Fatty acid	Methyl ester name	*M* (g/mol)	*N*	*T* (K)	μ_{exp} (mPa s)	μ_{cal} (mPa s)	*D* (%)
[38]	C10:0	Methyl caprate	186.2912	0	348.15	0.985	0.79	19.8
[38]	C12:0	Methyl laurate	214.3443	0	348.15	1.131	1.10	2.74
[38]	C14:0	Methyl myristate	242.3975	0	348.15	1.528	1.47	3.8
[1]	C16:1	Methyl palmitoleate	268.4348	1	283.15	6.43	6.20	3.58
					288.15	5.57	5.48	1.62
					293.15	4.83	4.86	−0.62
					298.15	4.27	4.34	−1.64
					303.15	3.81	3.88	−1.84
					308.15	3.4	3.48	−2.35
					313.15	3.13	3.14	−0.32
[38]	C18:0	Methyl stearate	298.5038	0	348.15	2.36	2.40	−1.69
[35]	C18:1	Methyl oleate	296.4879	1	303.15	4.88	4.91	−0.61
					333.15	2.62	2.70	−3.05
					363.15	1.64	1.64	0

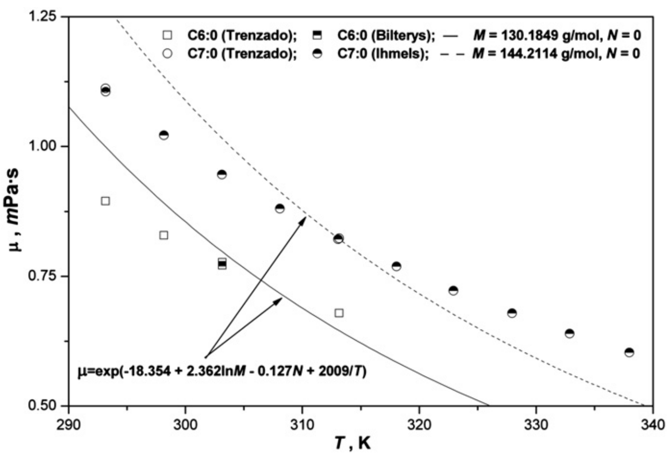


Fig. 6. Extrapolation for the dynamic viscosity of FAMEs.

The empirical model of viscosity was validated with experimental information reported in the literature; those data were not considered in the viscosity database compiled in this work. Table 7 shows the results for four saturated methyl esters and two mono-unsaturated methyl esters.

In order to prove the model capability for predictions, as well as its limitations, it was estimated the dynamic viscosity of the C6:0 and C7:0 methyl esters [36,37,39] by using Eq. (2). The results can be seen in Fig. 6, at which the symbols indicate the experimental measured viscosities, and lines indicate the corresponding calculated property.

3.3. Biodiesel's density

The FAME concentration of various individual biodiesel samples as well as binary biodiesel mixtures is reported in Table 8. The FAME distribution of some binary mixtures as coconut(1)+rapeseed(2), cotton(1)+babassu(2), and soybean(1)+babassu(2), were derived from the biodiesel concentration reported by Feitosa et al. [29] and Nogueira et al. [30]. It should be noted that biodiesel samples reported by Baroutian et al. [20], Veny et al. [21] and Hubber et al. [33] were originally characterized in mol fraction. Therefore, a conversion to mass fraction was carried out in this work by means of Eq. (3), and the results are shown in Table 8.

An extensive diversity on FAME concentration was considered in this work to test the developed models as can be seen on Table 8. For example, soybean, canola, and jatropha biodiesel samples are rich in unsaturated FAMEs (C18:1 and C18:2), whereas the coconut biodiesel is characterized by having abundance of short-chain saturated FAMEs (C12:0, C14:0 and C16:0).

Figs. 7 and 8 show deviations between the density that was estimated by the model and the experimental results reported in literature (for both biodiesel and biodiesel blends). Deviations were positive due the experimental density was always greater than calculated.

Statistical parameters for the empirical model of density (standard deviation (σ), average absolute deviation (*AAD*), number of experimental points (n_{exp}), and temperature range) are presented in Table 9. The model was tested with eighteen pure biodiesel samples (292 points), twenty binary biodiesel mixtures (185 points), and one ternary biodiesel blend (18 points) at different temperatures, representing a total of 495 experimental points. Smaller *AADs* were obtained in the Jatropha biodiesel reported by Veny et al. [21], whereas higher *AADs* were obtained in the biodiesel of Babassu reported by Nogueira et al. [30]. A standard deviation of 0.0037 and *AAD* of 0.43% was obtained for 495 experimental points. These results prove that the model can reproduce fairly near the experimental information. Likewise, these predictions are in the order of magnitude to those of the Group Contribution Model (GCM) proposed by Pratas et al. [7], who were obtained an average absolute deviation of 0.603% (original GCM), 2.69% (extended GCM), and 0.254% (revised GCM) for thirteen pure biodiesel samples, four binary biodiesel mixtures and one ternary biodiesel blend at different temperatures. In addition, our predictions were smaller than that reported by Anand et al. [22], who report an *AAD* of 1% for thirteen biodiesel samples tested.

3.4. Biodiesel's dynamic viscosity

The concentration profile used for the dynamic viscosity study is reported in Table 10. The mass fraction of the some biodiesel blends (coconut–colza, cotton–babassu, and soybean–babassu) was derived from the information provided by Feitosa et al. [29], and Nogueira et al. [30], who report the FAME content of individual biodiesel samples as well as the biodiesel content for the binary mixtures.

Figs. 9 and 10 show deviations between the dynamic viscosity model and experimental results reported in the literature (for both biodiesel and biodiesel blends). It can be seen that most of the deviations were positive and only few were negative.

The *AADs* for biodiesel and biodiesel blend systems studied in this work are reported in Table 11. Predicted values for nineteen biodiesel samples (164 points) and twenty four binary biodiesel mixtures (132 points), totalizing 296 experimental

Table 8
FAME concentration, in mass fraction (w), of various biodiesel samples (density study).

Reference	Biodiesel/FAME	C8:0	C10:0	C12:0	C14:0	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C20:1	C22:0	C22:1	C24:0
[29]	Coconut (Feitosa)	0.0408	0.0365	0.3535	0.1984	0.1383	–	0.0394	0.1430	0.0473	–	–	–	–	–	–
[29]	Soybean (Feitosa)	–	–	–	–	0.1132	–	–	0.2568	0.5494	0.0807	–	–	–	–	–
[29]	Colza (Feitosa)	–	–	–	–	0.0399	–	0.0391	0.5667	0.2361	0.0988	0.0194	–	–	–	–
[30]	Babassu (Nogueira)	–	0.051	0.2811	0.2556	0.1541	–	0.0504	0.2079	–	–	–	–	–	–	–
[30]	Cotton seed (Nogueira)	–	–	–	0.0062	0.2409	–	0.0256	0.1574	0.5699	–	–	–	–	–	–
[30]	Soybean (Nogueira)	–	–	–	–	0.1129	–	0.0396	0.1998	0.5839	0.0586	–	–	0.0052	–	–
[7]	Soybean-B (Pratas)	–	–	–	0.0007	0.1076	0.0007	0.0394	0.2296	0.5353	0.0702	0.0038	0.0023	0.008	0.0024	–
[7]	Rapeseed (Pratas)	–	0.0001	0.0004	0.0007	0.0522	0.002	0.0162	0.6211	0.2107	0.0695	0.0036	0.0135	0.0035	0.0019	0.0022
[7]	Palm (Pratas)	–	0.0003	0.0024	0.0057	0.4245	0.0013	0.0402	0.4192	0.098	0.0009	0.0003	0.0015	0.0009	–	0.0015
[7]	Sunflower (Patras)	–	–	0.0002	0.0007	0.064	0.0009	0.0422	0.2390	0.6416	0.0012	–	0.0015	0.0076	0.0008	–
[7]	Soybean-A (Pratas)	–	–	–	–	0.1704	–	0.0373	0.2863	0.5045	–	–	–	–	–	–
[20]	Palm (Baroutian)	–	–	–	–	0.41	–	0.04	0.45	0.1	–		–	–	–	–
[33]	Soybean-A (Hubber)	–	–	–	–	0.129	–	0.0891	0.3074	0.3841	0.0904	–	–	–	–	–
[33]	Soybean-B (Hubber)	–	–	–	–	0.1366	–	0.1241	0.3595	0.3136	0.0663	–	–	–	–	–
[21]	Jatropha (Veny)	–	–	–	–	0.1483	–	0.0716	0.4572	0.3229	–	–	–	–	–	–
[11]	Fish (Parente)	–	–	–	0.0376	0.0566	0.2809	0.0746	0.4229	0.1274	–	–	–	–	–	–
[11]	Sunflower (Parente)	–	–	–	–	0.071	–	0.048	0.226	0.655	–	–	–	–	–	–
[31]	Soybean (Mesquita)	–	–	–	–	0.1132	–	0.0313	0.2387	0.5494	0.0494	–	–	0.0181	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.0962$ (Feitosa)	0.0039	0.0035	0.034	0.0191	0.0494	–	0.0391	0.5259	0.2179	0.0893	0.0175	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.1967$ (Feitosa)	0.008	0.0072	0.0695	0.039	0.0593	–	0.0392	0.4834	0.199	0.0794	0.0156	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.397$ (Feitosa)	0.0162	0.0145	0.1403	0.0788	0.079	–	0.0392	0.3985	0.1611	0.0596	0.0117	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.4974$ (Feitosa)	0.0203	0.0182	0.1758	0.0987	0.0888	–	0.0392	0.356	0.1422	0.0497	0.0098	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.5977$ (Feitosa)	0.0244	0.0218	0.2113	0.1186	0.0987	–	0.0393	0.3135	0.1233	0.0397	0.0078	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.6952$ (Feitosa)	0.0284	0.0254	0.2458	0.1379	0.1083	–	0.0393	0.2721	0.1048	0.0301	0.0059	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.8039$ (Feitosa)	0.0328	0.0293	0.2842	0.1595	0.119	–	0.0393	0.2261	0.0843	0.0194	0.0038	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.9017$ (Feitosa)	0.0368	0.0329	0.3188	0.1789	0.1286	–	0.0394	0.1846	0.0659	0.0097	0.0019	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.166$ (Nogueira)	–	0.0425	0.2344	0.2142	0.1685	–	0.0463	0.1995	0.0946	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.196$ (Nogueira)	–	0.041	0.226	0.2067	0.1711	–	0.0455	0.198	0.1117	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.299$ (Nogueira)	–	0.0425	0.2344	0.2142	0.1685	–	0.0463	0.1995	0.0946	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.49$ (Nogueira)	–	0.026	0.1434	0.1334	0.1966	–	0.0382	0.1832	0.2793	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.684$ (Nogueira)	–	0.0161	0.0888	0.085	0.2135	–	0.0334	0.1734	0.3898	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.805$ (Nogueira)	–	0.0099	0.0548	0.0548	0.224	–	0.0304	0.1672	0.4588	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.9$ (Nogueira)	–	0.0051	0.0281	0.0311	0.2322	–	0.0281	0.1625	0.5129	–	–	–	–	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.099$ (Nogueira)	–	0.046	0.2533	0.2303	0.15	–	0.0493	0.2071	0.0578	0.0058	–	–	0.0005	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.297$ (Nogueira)	–	0.0359	0.1976	0.1797	0.1419	–	0.0472	0.2055	0.1734	0.0174	–	–	0.0015	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.404$ (Nogueira)	–	0.0304	0.1675	0.1523	0.1375	–	0.046	0.2046	0.2359	0.0237	–	–	0.0021	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.501$ (Nogueira)	–	0.0254	0.1403	0.1275	0.1335	–	0.045	0.2038	0.2925	0.0294	–	–	0.0026	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.605$ (Nogueira)	–	0.0201	0.111	0.101	0.1292	–	0.0439	0.203	0.3533	0.0355	–	–	0.0031	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.804$ (Nogueira)	–	0.01	0.0551	0.0501	0.121	–	0.0417	0.2014	0.4695	0.0471	–	–	0.0042	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.901$ (Nogueira)	–	0.005	0.0278	0.0253	0.117	–	0.0407	0.2006	0.5261	0.0528	–	–	0.0047	–	–
[7]	A. Soybean+Rapeseed (Pratas)	–	–	0.0003	0.0009	0.089	0.0015	0.0276	0.4182	0.3751	0.0702	0.0046	0.0068	0.0046	0.0012	–
[7]	Rapeseed+Palm (Pratas)	–	0.0002	0.002	0.0054	0.2309	0.0017	0.0302	0.5292	0.1547	0.0308	0.0049	0.0067	0.0024	0.0009	–
[7]	Soybean+Palm (Pratas)	–	0.0001	0.0018	0.0001	0.2556	0.0011	0.0404	0.3313	0.3172	0.0358	0.0039	0.002	0.0032	0.0012	0.0063
[7]	B. Soybean+Rapeseed (Pratas)	–	–	0.0002	0.0013	0.1057	0.0013	0.0266	0.4105	0.3667	0.071	0.0044	0.0067	0.0045	0.0012	–

data, are in close agreement with the measured data, with a global *AAD* of 6.39%. Minimum and maximum errors of 2.38 and 17.04% were obtained for the soybean($w_1=0.099$)+babassu($w_2=0.901$) binary system and colza biodiesel reported by Nogueira et al. [30] and Feitosa et al. [29], respectively (see Table 11). So, it can be established that the empirical model

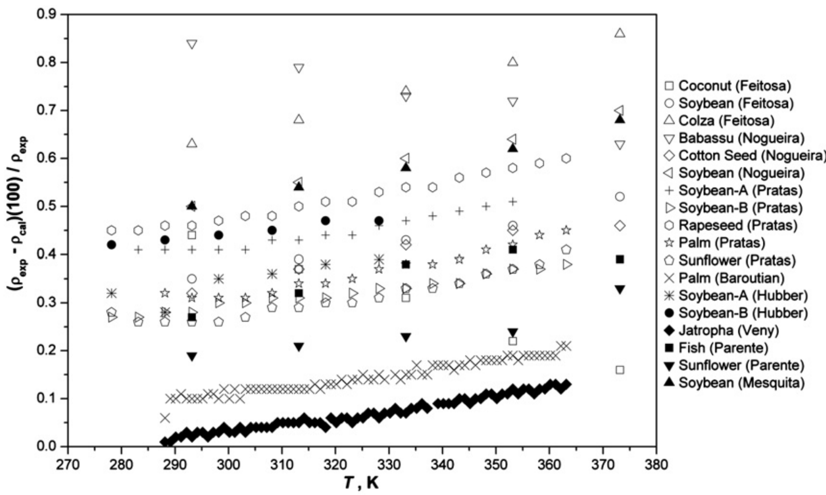


Fig. 7. Relative error for density (pure biodiesel samples).

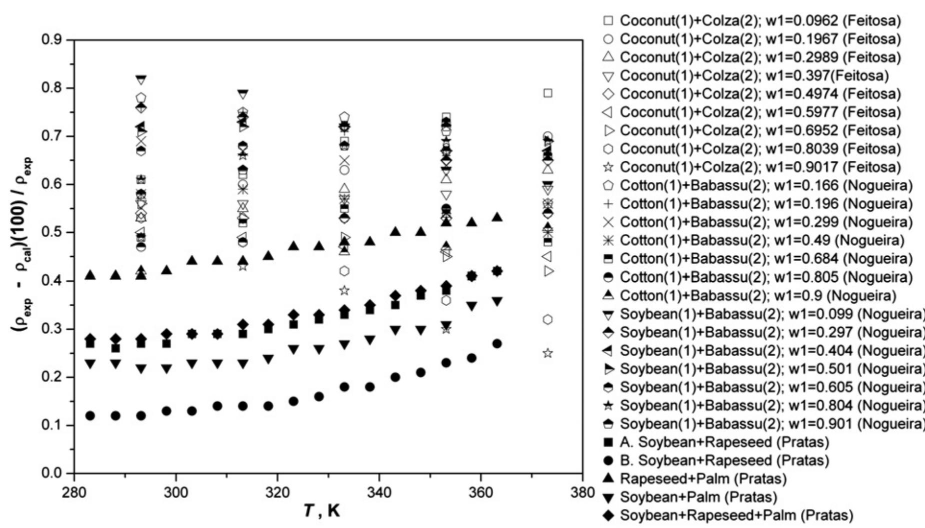


Fig. 8. Relative error for density (biodiesel blends).

Table 9
Statistical parameters for the empirical model developed in this work to predict the density of biodiesel.

Reference	Biodiesel	σ	*AAD* (%)	n_{exp}	Temperature range (K)
[29]	Coconut (Feitosa)	0.0027	0.30	5	[293.15, 373.15]
[29]	Soybean (Feitosa)	0.0037	0.43	5	[293.15, 373.15]
[29]	Colza (Feitosa)	0.0063	0.74	5	[293.15, 373.15]
[30]	Babassu (Nogueira)	0.0063	0.74	5	[293.15, 373.15]
[30]	Cotton seed (Nogueira)	0.0035	0.40	5	[293.15, 373.15]
[30]	Soybean (Nogueira)	0.0051	0.60	5	[293.15, 373.15]
[7]	Soybean-A (Pratas)	0.0038	0.45	15	[283.15, 353.15]
[7]	Soybean-B (Pratas)	0.0028	0.32	18	[278.15, 363.15]
[7]	Rapeseed (Pratas)	0.0044	0.52	18	[278.15, 363.15]
[7]	Palm (Pratas)	0.0031	0.37	16	[288.15, 363.15]
[7]	Sunflower (Patras)	0.0027	0.31	18	[278.15, 363.15]
[20]	Palm (Baroutian)	0.0012	0.14	75	[288.15, 363.15]
[33]	Soybean-A (Hubber)	0.003	0.35	6	[278.15, 328.15]
[33]	Soybean-B (Hubber)	0.0039	0.45	6	[278.15, 328.15]
[21]	Jatropha (Veny)	0.0006	0.07	75	[288.15, 363.15]
[11]	Fish (Parente)	0.003	0.35	5	[293.15, 373.15]
[11]	Sunflower (Parente)	0.0021	0.24	5	[293.15, 373.15]
[31]	Soybean (Mesquita)	0.005	0.58	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.0962$ (Feitosa)	0.0059	0.69	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.1967$ (Feitosa)	0.0054	0.64	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.2989$ (Feitosa)	0.005	0.58	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.397$ (Feitosa)	0.0048	0.57	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.4974$ (Feitosa)	0.0045	0.53	5	[293.15, 373.15]

Table 9 (*continued*)

Reference	Biodiesel	σ	*AAD* (%)	n_{exp}	Temperature range (K)
[29]	Coconut(1)+Colza(2); $w_1=0.5977$ (Feitosa)	0.0040	0.47	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.6952$ (Feitosa)	0.0042	0.49	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.8039$ (Feitosa)	0.0036	0.42	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); $w_1=0.9017$ (Feitosa)	0.0032	0.37	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); $w_1=0.166$ (Nogueira)	0.0061	0.71	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); $w_1=0.196$ (Nogueira)	0.0059	0.69	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); $w_1=0.299$ (Nogueira)	0.0055	0.64	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); $w_1=0.49$ (Nogueira)	0.0047	0.56	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); $w_1=0.684$ (Nogueira)	0.0044	0.52	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); $w_1=0.805$ (Nogueira)	0.0044	0.51	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); $w_1=0.9$ (Nogueira)	0.0039	0.46	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); $w_1=0.099$ (Nogueira)	0.0061	0.71	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); $w_1=0.297$ (Nogueira)	0.006	0.70	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); $w_1=0.404$ (Nogueira)	0.006	0.70	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); $w_1=0.501$ (Nogueira)	0.006	0.70	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); $w_1=0.605$ (Nogueira)	0.0059	0.69	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); $w_1=0.804$ (Nogueira)	0.0057	0.67	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); $w_1=0.901$ (Nogueira)	0.0056	0.65	4	[293.15, 353.15]
[7]	A. Soybean+Rapeseed (Pratas)	0.0028	0.32	18	[278.15, 363.15]
[7]	B. Soybean+Rapeseed (Pratas)	0.0015	0.17	18	[278.15, 363.15]
[7]	Rapeseed+Palm (Pratas)	0.004	0.46	18	[278.15, 363.15]
[7]	Soybean+Palm (Pratas)	0.0023	0.27	17	[283.15, 363.15]
[7]	Soybean+Rapeseed+Palm (Pratas)	0.0028	0.33	18	[278.15, 363.15]
	Total for pure biodiesel samples	**0.0035**	**0.41**	**292**	
	Total for biodiesel blends	**0.0047**	**0.54**	**203**	
	Total	**0.0041**	**0.48**	**495**	

Table 10
FAME concentration, in mass fraction, of various biodiesel samples (viscosity study).

Reference	Biodiesel/FAME	C8:0	C10:0	C12:0	C14:0	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C20:1	C22:0	C22:1	C24:0
[29]	Coconut (Feitosa)	0.0408	0.0365	0.3535	0.1984	0.1383	–	0.0394	0.1430	0.0473	–	–	–	–	–	–
[29]	Soybean (Feitosa)	–	–	–	–	0.1132	–	–	0.2568	0.5494	0.0807	–	–	–	–	–
[29]	Colza (Feitosa)	–	–	–	–	0.0399	–	0.0391	0.5667	0.2361	0.0988	0.0194	–	–	–	–
[30]	Babassu (Nogueira)	–	0.051	0.2811	0.2556	0.1541	–	0.0504	0.2079	–	–	–	–	–	–	–
[30]	Cotton Seed (Nogueira)	–	–	–	0.0062	0.2409	–	0.0256	0.1574	0.5699	–	–	–	–	–	–
[30]	Soybean (Nogueira)	–	–	–	–	0.1129	–	0.0396	0.1998	0.5839	0.0586	–	–	0.0052	–	–
[14]	Soybean (Yuan)	0.0002	–	–	0.0008	0.1049	0.0012	0.0427	0.242	0.5136	0.0748	0.0036	0.0028	0.004	0.0007	0.0014
[14]	Yellow grease (Yuan)	–	–	–	0.017	0.1947	0.000	0.1438	0.5467	0.0796	0.0069	0.0025	0.0052	0.0021	–	–
[14]	Coconut (Yuan)	0.092	0.064	0.487	0.17	0.077	–	0.022	0.054	0.022	–	–	–	–	–	–
[14]	Palm (Yuan)	–	–	–	–	0.406	–	0.051	0.4280	0.11	0.005	–	–	–	–	–
[14]	Canola (Yuan)	–	–	–	–	0.042	–	0.017	0.568	0.217	0.157	–	–	–	–	–
[11]	Fish (Parente)	–	–	–	0.0376	0.0566	0.2809	0.0746	0.4229	0.1274	–	–	–	–	–	–
[11]	Sunflower (Parente)	–	–	–	–	0.071	–	0.048	0.226	0.655	–	–	–	–	–	–
[15]	Soybean-A (Freitas)	–	–	–	–	0.1618	–	0.0382	0.288	0.5046	–	–	–	–	–	–
[15]	Soybean-B (Freitas)	–	–	–	0.0007	0.1078	0.0007	0.0395	0.2302	0.5366	0.0703	0.0038	0.0023	0.008	–	–
[15]	FAMEs standard (Freitas)	–	–	–	0.018	0.047	0.047	0.019	0.7113	0.0989	–	0.0589	–	–	–	–
[15]	Sunflower (Freitas)	–	–	0.0002	0.0007	0.0641	0.0009	0.0423	0.2393	0.6425	0.0012	–	0.0003	0.0077	0.0008	–
[15]	Rapeseed (Freitas)	–	0.0001	0.0004	0.0007	0.0526	0.002	0.0163	0.6249	0.2094	0.0699	0.006	0.0123	0.0135	0.0019	–
[15]	Palm (Freitas)	–	0.0003	0.0025	0.0057	0.4252	0.0013	0.0403	0.4199	0.0981	0.0009	0.0036	0.0015	0.0009	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.0962$ (Feitosa)	0.0039	0.0035	0.034	0.0191	0.0494	–	0.0391	0.5259	0.2179	0.0893	0.0175	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.1967$ (Feitosa)	0.008	0.0072	0.0695	0.039	0.0593	–	0.0392	0.4834	0.199	0.0794	0.0156	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.2989$ (Feitosa)	0.0122	0.0109	0.1057	0.0593	0.0693	–	0.0392	0.4401	0.1797	0.0693	0.0136	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.397$ (Feitosa)	0.0162	0.0145	0.1403	0.0788	0.079	–	0.0392	0.3985	0.1611	0.0596	0.0117	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.4974$ (Feitosa)	0.0203	0.0182	0.1758	0.0987	0.0888	–	0.0392	0.356	0.1422	0.0497	0.0098	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.5977$ (Feitosa)	0.0244	0.0218	0.2113	0.1186	0.0987	–	0.0393	0.3135	0.1233	0.0397	0.0078	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.6952$ (Feitosa)	0.0284	0.0254	0.2458	0.1379	0.1083	–	0.0393	0.2721	0.1048	0.0301	0.0059	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.8039$ (Feitosa)	0.0328	0.0293	0.2842	0.1595	0.119	–	0.0393	0.2261	0.0843	0.0194	0.0038	–	–	–	–
[29]	Coconut(1)+Colza(2); $w_1=0.9017$ (Feitosa)	0.0368	0.0329	0.3188	0.1789	0.1286	–	0.0394	0.1846	0.0659	0.0097	0.0019	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.166$ (Nogueira)	–	0.0425	0.2344	0.2142	0.1685	–	0.0463	0.1995	0.0946	–	–	–	–	–	–

Table 10 (*continued*)

Reference	Biodiesel/FAME	C8:0	C10:0	C12:0	C14:0	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C20:1	C22:0	C22:1	C24:0
[30]	Cotton(1)+Babassu(2); $w_1=0.196$ (Nogueira)	–	0.041	0.226	0.2067	0.1711	–	0.0455	0.198	0.1117	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.299$ (Nogueira)	–	0.0358	0.1971	0.181	0.1801	–	0.043	0.1928	0.1704	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.49$ (Nogueira)	–	0.026	0.1434	0.1334	0.1966	–	0.0382	0.1832	0.2793	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.684$ (Nogueira)	–	0.0161	0.0888	0.085	0.2135	–	0.0334	0.1734	0.3898	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.805$ (Nogueira)	–	0.0099	0.0548	0.0548	0.224	–	0.0304	0.1672	0.4588	–	–	–	–	–	–
[30]	Cotton(1)+Babassu(2); $w_1=0.9$ (Nogueira)	–	0.0051	0.0281	0.0311	0.2322	–	0.0281	0.1625	0.5129	–	–	–	–	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.099$ (Nogueira)	–	0.046	0.2533	0.2303	0.15	–	0.0493	0.2071	0.0578	0.0058	–	–	0.0005	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.297$ (Nogueira)	–	0.0359	0.1976	0.1797	0.1419	–	0.0472	0.2055	0.1734	0.0174	–	–	0.0015	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.404$ (Nogueira)	–	0.0304	0.1675	0.1523	0.1375	–	0.046	0.2046	0.2359	0.0237	–	–	0.0021	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.501$ (Nogueira)	–	0.0254	0.1403	0.1275	0.1335	–	0.045	0.2038	0.2925	0.0294	–	–	0.0026	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.605$ (Nogueira)	–	0.0201	0.111	0.101	0.1292	–	0.0439	0.203	0.3533	0.0355	–	–	0.0031	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.804$ (Nogueira)	–	0.01	0.0551	0.0501	0.121	–	0.0417	0.2014	0.4695	0.0471	–	–	0.0042	–	–
[30]	Soybean(1)+Babassu(2); $w_1=0.901$ (Nogueira)	–	0.005	0.0278	0.0253	0.117	–	0.0407	0.2006	0.5261	0.0528	–	–	0.0047	–	–
[15]	Soybean+Rapeseed (Freitas)	–	–	0.0002	0.0013	0.1057	0.0013	0.0266	0.4105	0.3667	0.071	0.0044	0.0067	0.0045	0.0012	–

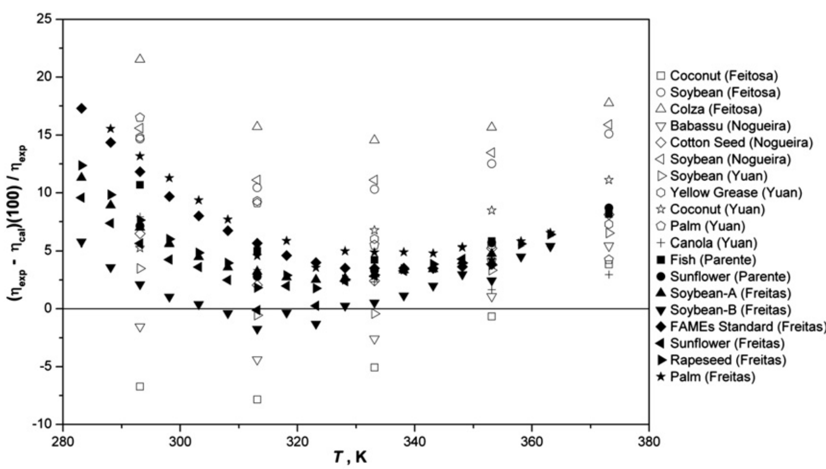


Fig. 9. Relative error for dynamic viscosity (pure biodiesel samples).

proposed in this work reproduces the experimental performance successfully, and it is comparable to the models tested by Feitosa et al. [15], who were obtaining an *AAD* of 8.07% (Ceriani's model), 5.34% (Yuan's model), 4.65% (revised Yuan's model) and 7.25% (Krisnangkura's model), for twenty two biodiesel samples, fourteen mixtures of FAMEs and one binary biodiesel mixture. Also our model are in the order of magnitude of the models tested by do Carmo et al. [19] who were obtaining an average absolute deviation of 10.61% (Ceriani's model), 7.66% (Yuan's model), 7% (revised Yuan's model), 7.59% (one-fluid do Carmo's model), and 6.66% (two-fluid do Carmo's model), for thirty one biodiesel samples and four binary biodiesel mixtures (totalizing 193 experimental data).

It is important to emphasize that the prediction models developed in this work for both the density and viscosity, represented by Eqs. (7) and (8), should not be used with the castor biodiesel, as well as in any blend containing the castor biodiesel, due to that biodiesel consists mainly of an hydroxilated FAME (about 90%) according to Knothe [4], and this particular FAME was not included in the database of this work. Although colza biodiesel (Tables 8, 9, 10 and 11) is better known as rapeseed biodiesel, we decided to use the original name that was reported by Feitosa et al. [29].

4. Conclusions

We develop empirical models to predict the density and dynamic viscosity for both methyl esters and biodiesel samples.

The parameters of each model were adjusted using a two-level-factorial method. The analysis of variance (ANOVA) showed that all parameters were significant. Validation of the empirical models was done by using experimental data not included to adjust the parameters.

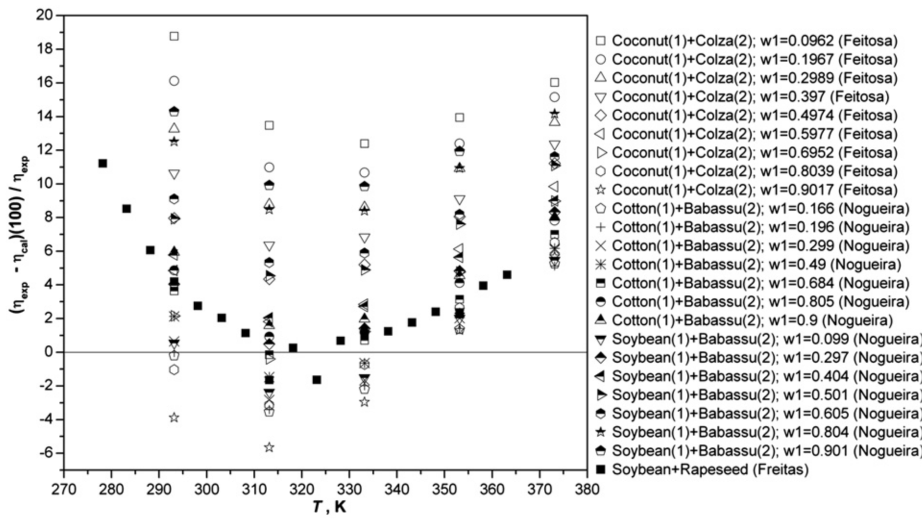


Fig. 10. Relative error for dynamic viscosity (biodiesel blends).

Table 11
Statistical parameters for the empirical model developed in this work to predict the dynamic viscosity of biodiesel.

Reference	Biodiesel	σ	*AAD* (%)	n_{exp}	Temperature range (K)
[29]	Coconut (Feitosa)	0.15	4.83	5	[293.15, 373.15]
[29]	Soybean (Feitosa)	0.50	12.60	5	[293.15, 373.15]
[29]	Colza (Feitosa)	0.83	17.04	5	[293.15, 373.15]
[30]	Babassu (Nogueira)	0.07	3.01	5	[293.15, 373.15]
[30]	Cotton seed (Nogueira)	0.19	4.86	5	[293.15, 373.15]
[30]	Soybean (Nogueira)	0.54	13.43	5	[293.15, 373.15]
[14]	Soybean (Yuan)	0.10	2.86	5	[293.15, 373.15]
[14]	Yellow grease (Yuan)	0.51	8.57	5	[293.15, 373.15]
[14]	Coconut (Yuan)	0.13	7.42	5	[293.15, 373.15]
[14]	Palm (Yuan)	0.55	7.91	5	[293.15, 373.15]
[14]	Canola (Yuan)	0.23	3.66	5	[293.15, 373.15]
[11]	Fish (Parente)	0.32	6.77	5	[293.15, 373.15]
[11]	Sunflower (Parente)	0.21	5.52	5	[293.15, 373.15]
[15]	Soybean–A (Freitas)	0.33	4.71	15	[283.15, 353.15]
[15]	Soybean-B (Freitas)	0.21	2.45	18	[278.15, 363.15]
[15]	FAMEs standard (Freitas)	0.60	6.91	15	[283.15, 353.15]
[15]	Sunflower (Freitas)	0.25	4.03	17	[283.15, 363.15]
[15]	Rapeseed (Freitas)	0.52	5.50	18	[278.15, 363.15]
[15]	Palm (Freitas)	0.45	7.03	16	[288.15, 363.15]
[29]	Coconut(1)+Colza(2); w_1=0.0962 (Feitosa)	0.68	14.93	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.1967 (Feitosa)	0.54	13.07	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.2989 (Feitosa)	0.42	11.05	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.397 (Feitosa)	0.31	9.06	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.4974 (Feitosa)	0.22	7.36	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.5977 (Feitosa)	0.13	5.10	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.6952 (Feitosa)	0.07	3.51	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.8039 (Feitosa)	0.06	2.81	5	[293.15, 373.15]
[29]	Coconut(1)+Colza(2); w_1=0.9017 (Feitosa)	0.10	3.90	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); w_1=0.166 (Nogueira)	0.06	2.51	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); w_1=0.196 (Nogueira)	0.06	2.39	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); w_1=0.299 (Nogueira)	0.06	2.65	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); w_1=0.49 (Nogueira)	0.06	2.55	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); w_1=0.684 (Nogueira)	0.10	2.93	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); w_1=0.805 (Nogueira)	0.14	3.79	5	[293.15, 373.15]
[30]	Cotton(1)+Babassu(2); w_1=0.9 (Nogueira)	0.17	4.42	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); w_1=0.099 (Nogueira)	0.05	2.38	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); w_1=0.297 (Nogueira)	0.11	3.82	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); w_1=0.404 (Nogueira)	0.15	5.03	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); w_1=0.501 (Nogueira)	0.23	7.21	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); w_1=0.605 (Nogueira)	0.27	8.03	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); w_1=0.804 (Nogueira)	0.40	10.89	5	[293.15, 373.15]
[30]	Soybean(1)+Babassu(2); w_1=0.901 (Nogueira)	0.52	11.51	4	[293.15, 353.15]
[15]	Soybean+Rapeseed (Freitas)	0.32	2.72	18	[278.15, 363.15]
	Total for pure biodiesel samples	**0.35**	**6.80**	**164**	
	Total for biodiesel blends	**0.22**	**5.98**	**132**	
	Total	**0.29**	**6.39**	**296**	

Capability of the empirical models (extrapolation) was done by estimating properties for methyl esters of relative low molecular weight as methyl hexanoate and methyl heptanoate.

The empirical models represent and correctly reproduce the behaviors of the real physical properties of methyl ester compounds.

The results suggest a relationship between molecular weight, fatty acid methyl ester type (saturated or unsaturated), and temperature, as independent variables; and each one of the density and dynamic viscosity, as dependent variables.

Mixing rules in conjunction with empirical models of FAMEs were used to successfully predict the density and viscosity of biodiesel.

An interesting future study might involve predicting other physical properties of biodiesel following a similar methodology to that used in this work.

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Appendix

Some examples illustrating how empirical models can be used to predict the density and viscosity of some methyl esters and biodiesel samples are provided.

Example 1. Pratas et al. 2010 [6] report that the density of methyl linoleate is 0.8715 g/cm^3 at 313.15 K. Compare the results with the value estimated by Eq. (1).

Solution. From Table 1, M=294.4721 g/mol, N=2.
With Eq. (1),

$$\rho = 1.069 + \frac{3.575}{294.4721} + 0.0113(2) - 7.41\times10^{-4}(313.15)$$
$$= 0.8717\ \frac{g}{cm^3}$$

$$\text{Error} = \frac{0.8715-0.8717}{0.8715}\times100 = -0.02\%$$

Example 2. Use the method developed in this work to estimate the density of palm biodiesel at 353.15 K. The experimental value is reported to be 0.8288 g/cm^3 [20].

Solution. The molecular weight and number of double bonds of FAMEs reported in Table 1, as well as the FAME composition from Table 8 are used. With Eq. (7),

$$\rho_b = 0.41\left(1.069 + \frac{3.575}{270.4507} + 0.0113(0) - 7.41\times10^{-4}(353.15)\right)$$
$$+0.04\left(1.069 + \frac{3.575}{298.5038} + 0.0113(0) - 7.41\times10^{-4}(353.15)\right)$$
$$+0.45\left(1.069 + \frac{3.575}{296.4879} + 0.0113(1) - 7.41\times10^{-4}(353.15)\right)$$
$$+0.1\left(1.069 + \frac{3.575}{294.4721} + 0.0113(2) - 7.41\times10^{-4}(353.15)\right)$$
$$= 0.8272\ \frac{g}{cm^3}$$

$$\text{Error} = \frac{0.8288-0.8272}{0.8288}\times100 = 0.19\%$$

Example 3. Estimate the dynamic viscosity for the methyl oleate compound at 333.15 K by means of the empirical method developed in this work. After that, compare with the value (2.6377 mPa s) reported by Pratas et al. [6].

Solution. From Table 2, M=296.4879 g/mol, N=1.
With Eq. (2),

$$\mu = \exp\left(-18.354 + 2.362\ \ln(296.4879) - 0.127(1) + \frac{2009}{333.15}\right)$$
$$= 2.7016\ \text{mPa s}$$

$$\text{Error} = \frac{2.6377-2.7016}{2.6377}\times100 = -2.42\%$$

Example 4. Calculate the dynamic viscosity of fish biodiesel at 353.15 K. The literature value for the viscosity at this temperature is 1.8580 mPa s [11].

Solution. From Table 2 and Table 10, the molecular weight, number of double bonds, and FAME composition are used. With Eq. (8),

$$\mu_b = 0.0376\left[\exp\left(-18.354 + 2.362\ \ln(242.3975) - 0.127(0) + \frac{2009}{353.15}\right)\right]$$
$$+0.0566\left[\exp\left(-18.354 + 2.362\ \ln(270.4507) - 0.127(0) + \frac{2009}{353.15}\right)\right]$$
$$+0.2809\left[\exp\left(-18.354 + 2.362\ \ln(268.4348) - 0.127(1) + \frac{2009}{353.15}\right)\right]$$
$$+0.0746\left[\exp\left(-18.354 + 2.362\ \ln(298.5038) - 0.127(0) + \frac{2009}{353.15}\right)\right]$$
$$+0.4229\left[\exp\left(-18.354 + 2.362\ \ln(296.4879) - 0.127(1) + \frac{2009}{353.15}\right)\right]$$
$$+0.1274\left[\exp\left(-18.354 + 2.362\ \ln(294.4721) - 0.127(2) + \frac{2009}{353.15}\right)\right]$$
$$= 1.7659\ \text{mPa s}$$

$$\text{Error} = \frac{1.858-1.7659}{1.7659}\times100 = -5.22\%$$

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